

ELECTRONIC SUPPLEMENTARY INFORMATION

Experimental and theoretical studies on fluvastatin primary photoproducts formation

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Determination of the fluvastatin molar absorption coefficient

The molar absorption coefficient (ϵ) was determined using Lambert-Beer's law:

$$A = \epsilon l c$$

- A absorbance at the maximum absorption of fluvastatin (302 nm),
 l path length of the radiation beam [cm], in our experiment $l = 0.2$ cm,
 c fluvastatin concentration [mol/dm³] which for the tested samples is shown in Table 1.

Table.1 Concentration of the fluvastatin tested samples

Sample number	Mass of FLV [mg]	n [mol]	V [dm ³]	c [mol/ dm ³]
1	1.201	2.77066E-06	0.01	0.000277
2	1.204	2.77759E-06	0.01	0.000278
3	1.21	2.79143E-06	0.01	0.000279
4	1.205	2.77989E-06	0.01	0.000278
5	1.204	2.77759E-06	0.01	0.000278

Molar absorption coefficients were calculated for each sample. Average molar absorption coefficient at $\lambda = 302$ nm was estimated to be 11800 ± 1000 [M⁻¹ cm⁻¹].

Using the resulting value $\epsilon_{302\text{nm}}$, molar absorption coefficient for the whole UV spectrum was calculated.

Determination of the fluvastatin quantum yield

Table 2. The parameters used for calculating of the fluvastatin quantum yield.

Sample number	Peak area	c_n [mol/ dm ³]	Δc_n [mol/ dm ³]	I_a [molquantum/ dm ³ ·s]	Φ
0	19630.2	0.00278	0	0.000245547	0
1	15828.8	0.002242	0.000538349	0.000229347	0.117366
2	12563.8	0.001779	0.001000733	0.0002121	0.117955
3	9852.4	0.001395	0.001384718	0.000215947	0.106872
4	7638.3	0.001082	0.001698275	0.00020731	0.102399
5	6493.3	0.00092	0.001860386	0.000190502	0.097657

Mass spectra of the studied compounds

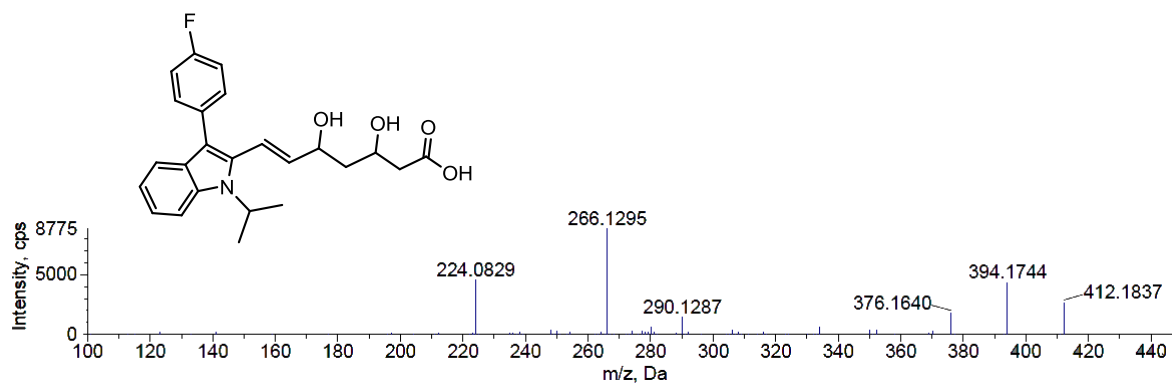


Fig. S1. Positive ions MS/MS spectrum of fluvastatin

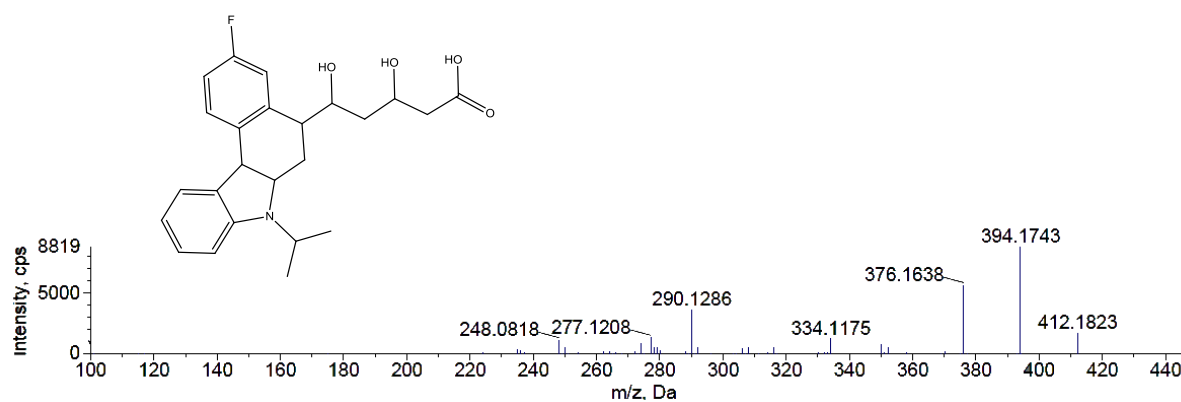


Fig.S2. Positive ions MS/MS spectrum of FP1

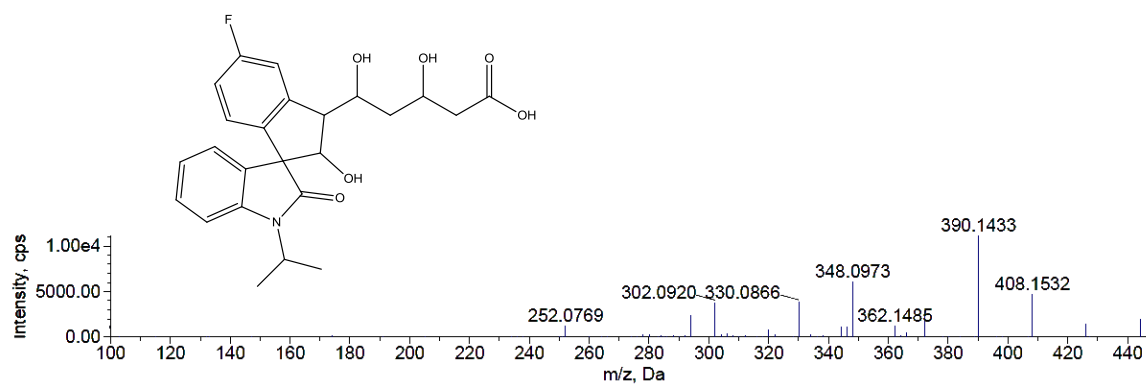


Fig.S3. Positive ions MS/MS spectrum of FP2a

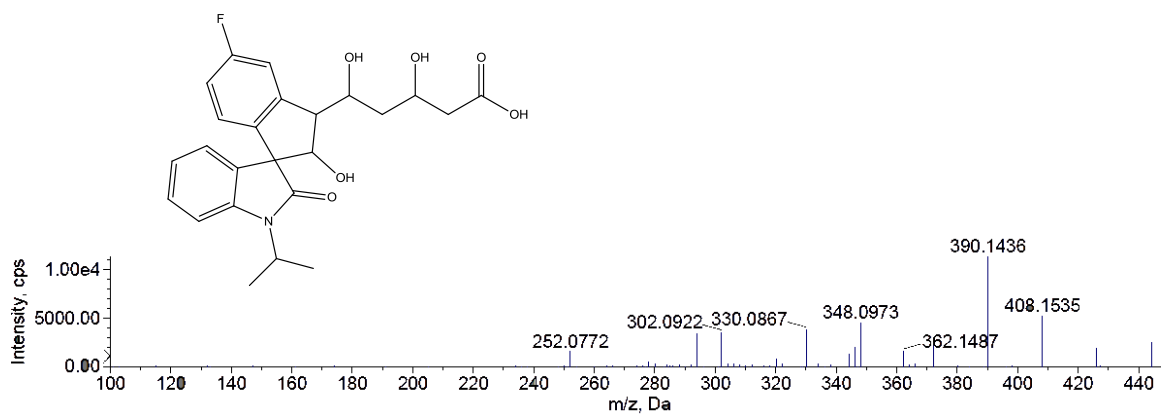


Fig.S4. Positive ions MS/MS spectrum of FP2b

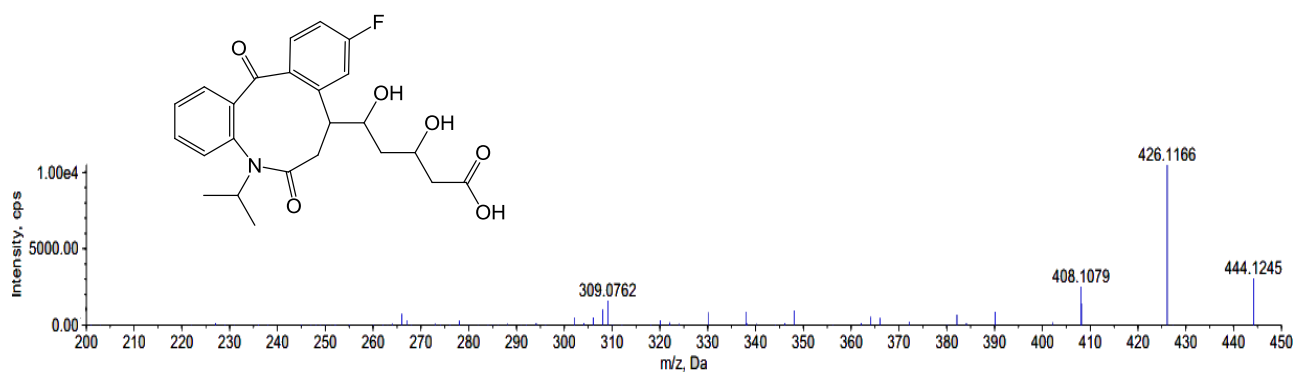


Fig.S5. Positive ions MS/MS spectrum of FP5

Energy profile of mechanism for FP1 formation (pathway B)

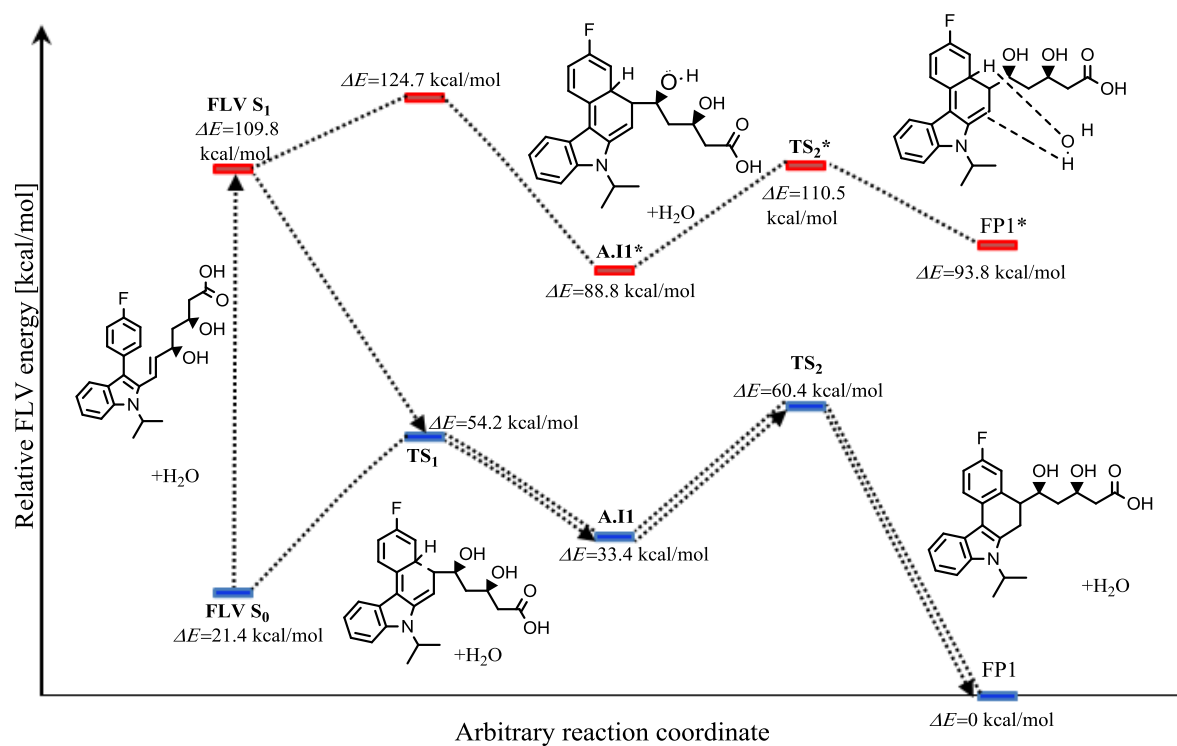
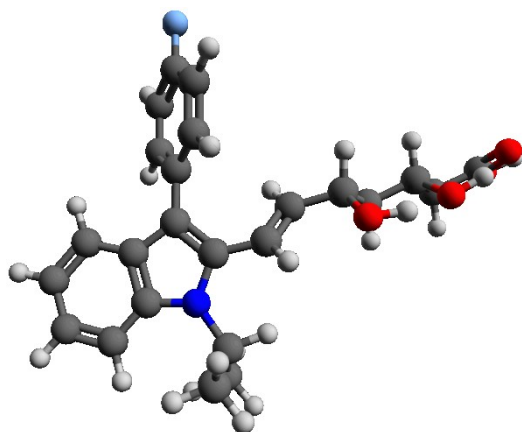
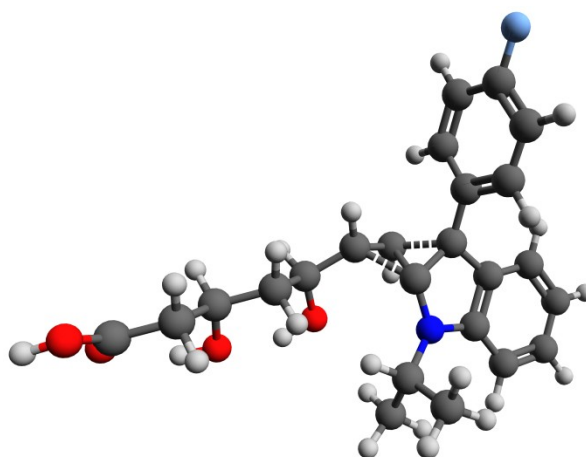


Fig. S6. Energy profile of mechanism for FP1 formation (pathway B)

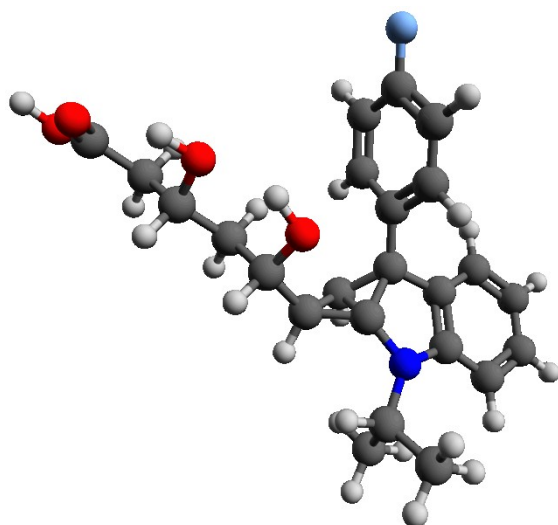
Structures of intermediates and transition states of FP2a and FP2b



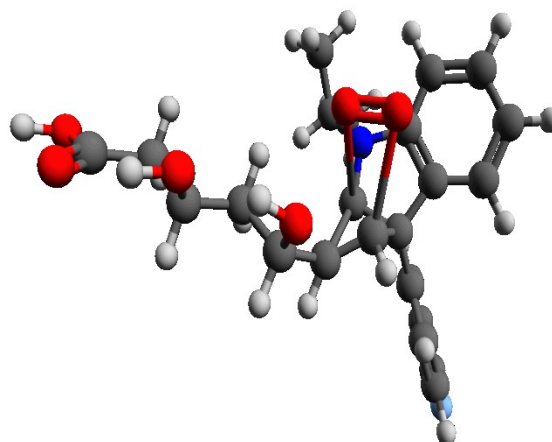
FLV



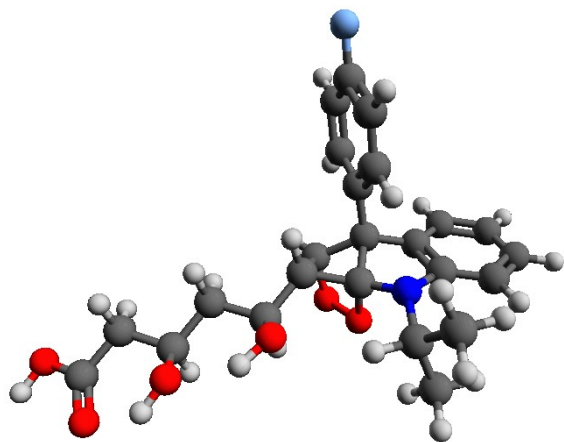
TS₁



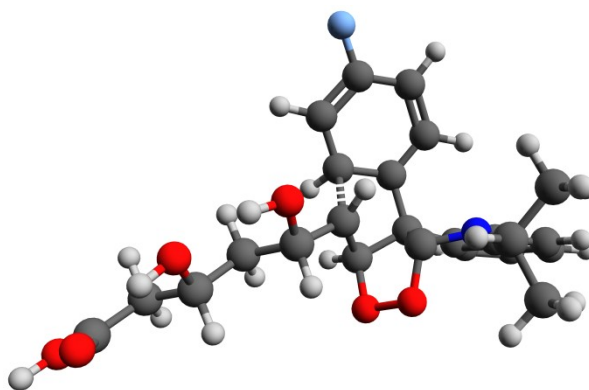
II



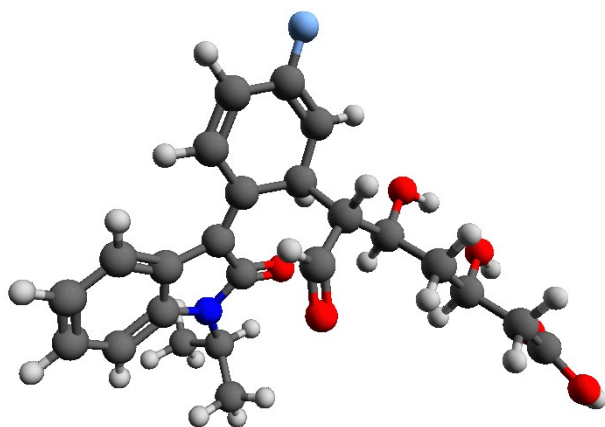
TS₂



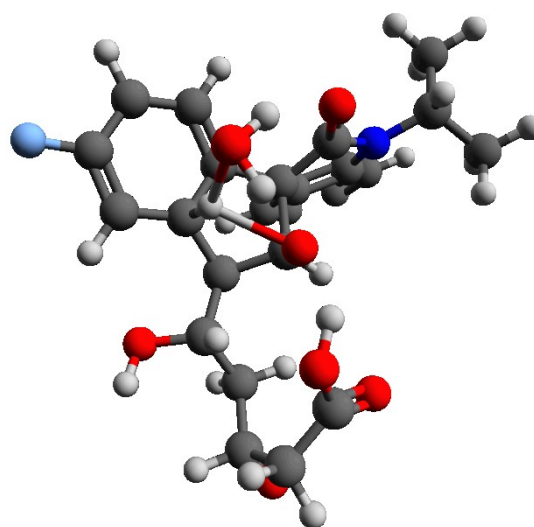
I2



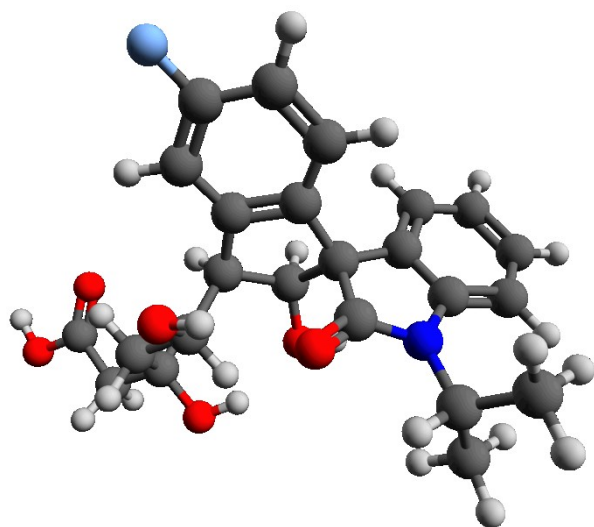
TS₃



I3

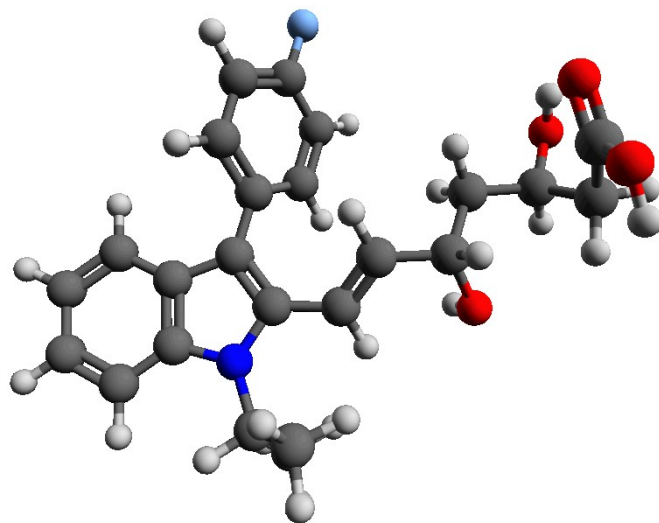


TS₄

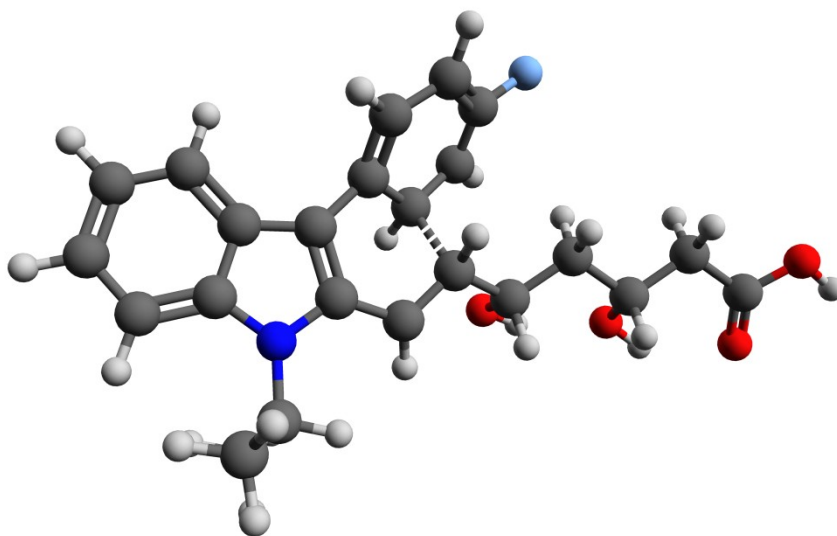


FP2a, FP2b

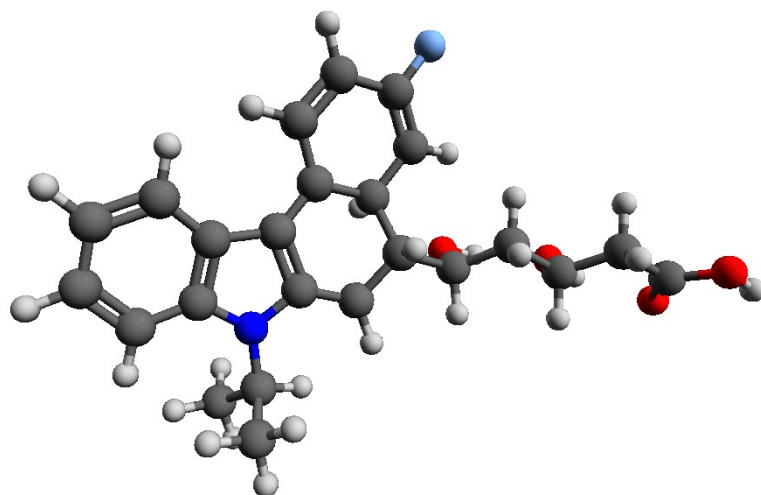
Structures of intermediates and transition states of FP1 (pathway A)



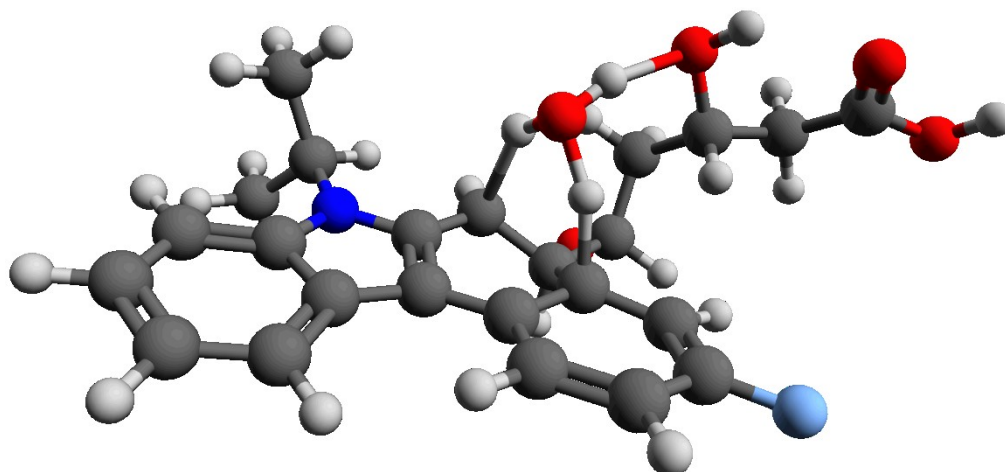
FLV – conformer A



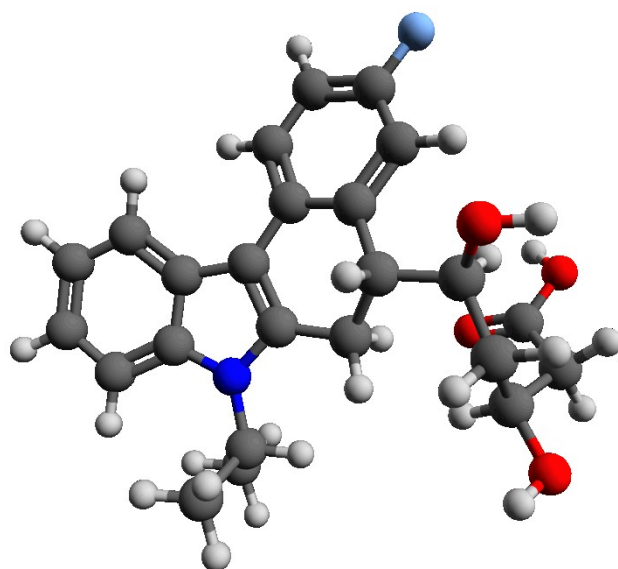
A.TS₁



A.I1

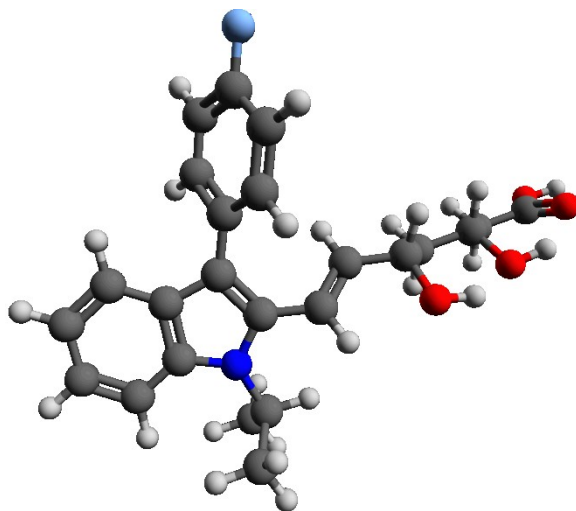


A.TS₂

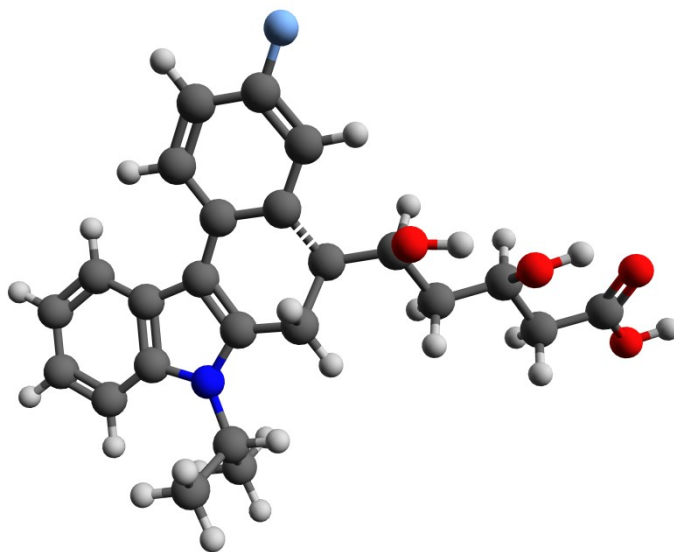


FP1

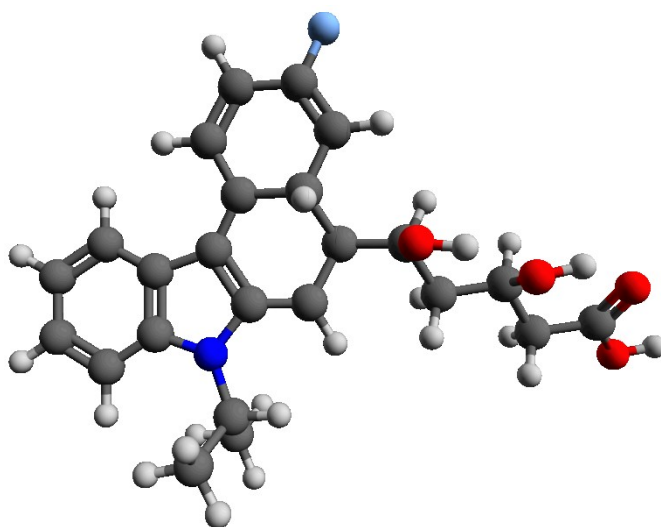
Structures of intermediates and transition states of FP1 (pathway B)



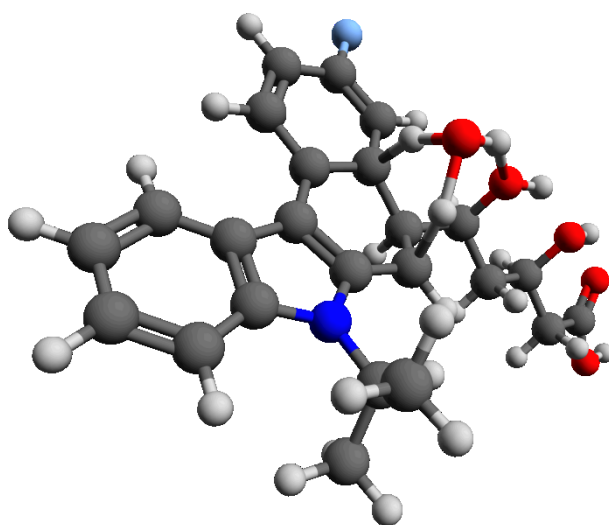
FLV-conformer B



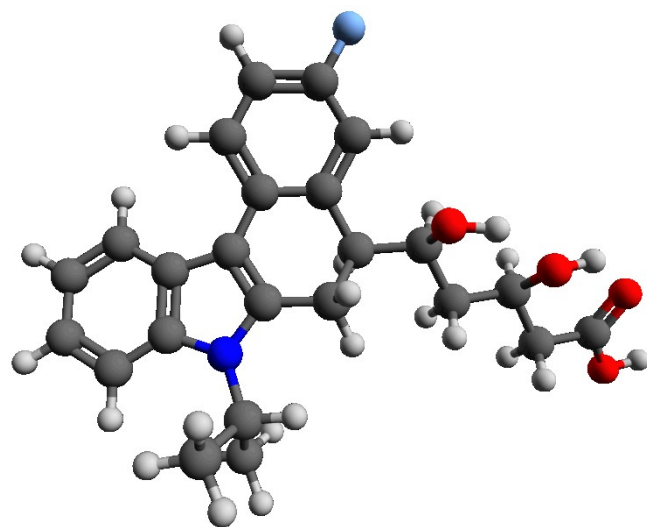
B.TS₁



B.I1



B.TS₂



FP1

Cartesian coordinates of the studied structures

1. FLV (conformer A)

6	-4.448215000	2.059776000	-0.276026000
6	-5.819598000	1.942394000	-0.408114000
6	-6.432637000	0.679303000	-0.422706000
6	-5.689662000	-0.484639000	-0.308873000
6	-4.303189000	-0.368900000	-0.166383000
6	-3.673916000	0.899911000	-0.143667000
7	-3.316570000	-1.331682000	-0.057081000
6	-2.081879000	-0.696538000	0.021898000
6	-2.264756000	0.673422000	-0.029690000
6	-1.218759000	1.703269000	-0.001940000
6	-1.291414000	2.766166000	0.906056000
6	-0.274617000	3.711871000	0.995574000
6	0.821574000	3.571304000	0.167174000
6	0.927831000	2.553036000	-0.764785000
6	-0.105460000	1.631675000	-0.850176000
6	-3.518670000	-2.773742000	0.103973000
6	-4.411698000	-3.093264000	1.294368000
6	-3.995242000	-3.411091000	-1.192718000
9	1.843552000	4.456209000	0.282308000
6	-0.839899000	-1.453322000	0.104010000
6	0.219571000	-1.079433000	0.827496000
6	1.545271000	-1.764943000	0.788471000
6	2.580872000	-0.840590000	0.129754000
6	4.007267000	-1.318004000	0.317385000
6	5.001188000	-0.398990000	-0.375719000
6	6.412345000	-0.869428000	-0.210317000
8	7.306793000	0.043086000	-0.616657000

8	1.423666000	-2.981931000	0.102135000
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1	-6.183375000	-1.453544000	-0.345560000
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1	1.821070000	2.477535000	-1.381320000
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1	-4.436495000	-4.178219000	1.456230000
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1	2.499692000	0.183985000	0.526681000
1	2.343116000	-0.787527000	-0.946012000
1	4.235457000	-1.331994000	1.401189000
1	4.781376000	-0.371985000	-1.454923000
1	4.907094000	0.639238000	-0.024899000
1	8.184312000	-0.361857000	-0.494078000
1	2.333084000	-3.277666000	-0.083369000
1	5.007870000	-2.937234000	0.001930000
8	6.752668000	-1.950757000	0.227190000

8	4.095821000	2.692256000	-0.207477000
1	4.750021000	3.196728000	-0.705417000
1	3.488361000	3.361794000	0.141019000

2. TS₁ (pathway A)

6	4.815981000	2.093174000	0.295909000
6	6.177111000	1.915734000	0.448074000
6	6.752517000	0.636117000	0.353645000
6	5.980886000	-0.489561000	0.107250000
6	4.602368000	-0.321785000	-0.040716000
6	4.007498000	0.971973000	0.046675000
7	3.595325000	-1.241857000	-0.264013000
6	2.388675000	-0.560730000	-0.319346000
6	2.620582000	0.807116000	-0.169578000
6	1.450737000	1.689703000	-0.099459000
6	1.155254000	2.669672000	-1.001921000
6	-0.111485000	3.317018000	-1.001042000
6	-1.022593000	2.967676000	-0.028625000
6	-0.761724000	1.990358000	0.922433000
6	0.368053000	1.144959000	0.739949000
6	3.725710000	-2.688717000	-0.427427000
6	4.626174000	-3.051327000	-1.599410000
6	4.148530000	-3.350083000	0.876237000
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6	-0.042327000	-0.246212000	-0.239181000
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6	-2.627702000	-0.226021000	-0.183294000
6	-3.817992000	-1.164569000	-0.134139000
6	-5.108259000	-0.443770000	-0.498708000

6	-6.296852000	-1.349555000	-0.445855000
8	-7.385554000	-0.809581000	-1.033058000
8	-1.244911000	-1.113274000	1.620620000
8	-3.897631000	-1.694196000	1.178062000
1	4.361447000	3.081006000	0.367070000
1	6.816711000	2.774841000	0.643157000
1	7.828143000	0.523465000	0.478086000
1	6.446325000	-1.471526000	0.052590000
1	1.906304000	2.968436000	-1.733065000
1	-0.343519000	4.120524000	-1.695067000
1	-1.445083000	1.839032000	1.754057000
1	0.685598000	0.636110000	1.652551000
1	2.710863000	-3.030700000	-0.675549000
1	5.671314000	-2.773943000	-1.418408000
1	4.295891000	-2.545290000	-2.514057000
1	4.594729000	-4.134568000	-1.771547000
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1	-2.533806000	0.172476000	-1.206000000
1	-2.826383000	0.628003000	0.478668000
1	-3.655121000	-1.989916000	-0.855335000
1	-5.307950000	0.381922000	0.204872000
1	-5.047969000	0.010169000	-1.498226000
1	-8.107313000	-1.453742000	-0.914017000
1	-2.094642000	-1.507720000	1.886287000

1	-4.637247000	-2.326662000	1.176420000
8	-6.333223000	-2.448200000	0.064063000
8	-7.271363000	1.678288000	0.515138000
1	-7.091075000	2.554707000	0.154853000
1	-7.585768000	1.159373000	-0.238785000

3. A.II (pathway A)

6	4.982477000	1.378719000	-0.827406000
6	6.277889000	0.917887000	-1.044700000
6	6.589773000	-0.419947000	-0.821447000
6	5.626888000	-1.320697000	-0.372650000
6	4.334525000	-0.855517000	-0.145877000
6	3.996449000	0.501938000	-0.382904000
7	3.215890000	-1.552721000	0.300328000
6	2.106695000	-0.703772000	0.236120000
6	2.581620000	0.643387000	-0.071238000
6	1.714962000	1.695961000	0.036798000
6	2.062641000	3.051193000	-0.280964000
6	1.161682000	4.057386000	-0.205549000
6	-0.183202000	3.776844000	0.224757000
6	-0.603492000	2.561822000	0.583978000
6	0.336632000	1.395966000	0.624928000
6	3.095143000	-2.991509000	0.498587000
6	3.174516000	-3.746252000	-0.821695000
6	4.060191000	-3.524769000	1.549403000
9	-1.010666000	4.833760000	0.259612000
6	0.794459000	-1.001632000	0.305677000
6	-0.214909000	0.089033000	0.039871000
6	-1.608697000	-0.316053000	0.547029000
6	-2.763272000	0.237295000	-0.292031000

6	-4.095191000	-0.397666000	0.056677000
6	-5.208887000	0.096905000	-0.854491000
6	-6.537177000	-0.501878000	-0.507889000
8	-7.463708000	-0.260034000	-1.434956000
8	-1.707598000	0.021391000	1.907542000
8	-4.388924000	-0.081587000	1.411260000
1	4.754548000	2.422620000	-1.030052000
1	7.042772000	1.605233000	-1.400154000
1	7.601923000	-0.777638000	-1.003779000
1	5.891391000	-2.363291000	-0.220324000
1	3.071867000	3.268225000	-0.620324000
1	1.416706000	5.083395000	-0.460560000
1	-1.604004000	2.431161000	0.984560000
1	0.498905000	1.160811000	1.700872000
1	2.086792000	-3.127168000	0.913808000
1	4.157039000	-3.615721000	-1.294673000
1	2.413172000	-3.377249000	-1.520849000
1	3.013421000	-4.821010000	-0.666947000
1	5.098397000	-3.554175000	1.200161000
1	3.779523000	-4.551678000	1.816136000
1	4.024283000	-2.910423000	2.456498000
1	0.436646000	-2.028423000	0.383031000
1	-0.305200000	0.216704000	-1.062369000
1	-1.670385000	-1.421403000	0.425925000
1	-2.555580000	0.035038000	-1.354100000
1	-2.849587000	1.328429000	-0.185258000
1	-4.018867000	-1.494771000	-0.067601000
1	-5.299266000	1.191841000	-0.777047000
1	-4.996051000	-0.132843000	-1.907154000

1	-8.284481000	-0.687587000	-1.130444000
1	-2.647179000	-0.069537000	2.149761000
1	-5.220189000	-0.542491000	1.622325000
8	-6.784886000	-1.136275000	0.503744000
8	-5.659228000	-3.120554000	-1.180274000
1	-6.037790000	-3.031819000	-0.294387000
1	-5.269571000	-4.002421000	-1.204300000

4. TS₂ (pathway A)

6	-3.871268000	2.386954000	-0.310019000
6	-5.204522000	2.353852000	-0.712593000
6	-5.862858000	1.141718000	-0.891950000
6	-5.206563000	-0.065815000	-0.651788000
6	-3.881202000	-0.028396000	-0.241693000
6	-3.180703000	1.195290000	-0.087953000
7	-3.019729000	-1.084087000	0.084182000
6	-1.780119000	-0.576946000	0.420639000
6	-1.834592000	0.852799000	0.318218000
6	-0.644883000	1.586509000	0.407049000
6	-0.561244000	2.972088000	0.069908000
6	0.602433000	3.678487000	0.187270000
6	1.764507000	3.038237000	0.665596000
6	1.765009000	1.712856000	0.961411000
6	0.607825000	0.895869000	0.704942000
6	-3.319752000	-2.509549000	0.012500000
6	-4.469580000	-2.910161000	0.926760000
6	-3.511597000	-2.960291000	-1.429230000
9	2.871428000	3.779575000	0.841961000
6	-0.612020000	-1.275683000	0.695682000
6	0.447769000	-0.453961000	1.419171000

6	1.724978000	-1.279550000	1.663646000
6	2.329582000	-1.986280000	0.446715000
6	3.226181000	-1.126671000	-0.438733000
6	4.697045000	-1.305373000	-0.089118000
6	5.593942000	-0.450093000	-0.935780000
8	6.774813000	-0.215180000	-0.359221000
8	1.324774000	-2.250240000	2.617219000
8	2.983842000	-1.487505000	-1.796127000
1	-3.393426000	3.351908000	-0.152089000
1	-5.733737000	3.289556000	-0.885659000
1	-6.902507000	1.127936000	-1.214357000
1	-5.734131000	-1.006320000	-0.791653000
1	-1.453863000	3.481467000	-0.281340000
1	0.652142000	4.735291000	-0.067704000
1	2.677669000	1.281787000	1.370114000
1	0.734061000	0.445273000	-0.677319000
1	-2.419698000	-3.005393000	0.397871000
1	-5.432885000	-2.510114000	0.591171000
1	-4.292931000	-2.551815000	1.947616000
1	-4.556998000	-4.003906000	0.954233000
1	-4.380942000	-2.478391000	-1.894017000
1	-3.661996000	-4.046585000	-1.475855000
1	-2.627594000	-2.706958000	-2.028406000
1	-0.659170000	-2.328563000	0.975361000
1	0.107156000	-0.229168000	2.454235000
1	2.495113000	-0.621378000	2.116683000
1	1.514942000	-2.404802000	-0.159305000
1	2.910685000	-2.855173000	0.797579000
1	2.980518000	-0.058238000	-0.310539000

1	4.877959000	-1.089382000	0.972995000
1	4.984445000	-2.356253000	-0.253308000
1	7.294530000	0.320020000	-0.986643000
1	2.096145000	-2.785871000	2.844253000
1	3.624323000	-0.970856000	-2.325573000
8	5.305651000	-0.023551000	-2.035784000
8	0.526203000	-0.283112000	-1.649155000
1	1.373554000	-0.744735000	-1.889793000
1	-0.010578000	-0.945542000	-1.074811000

5. FP1 (pathway A)

6	4.151716000	2.044336000	-0.041165000
6	5.508252000	1.778002000	0.029141000
6	5.978451000	0.459762000	0.101119000
6	5.102776000	-0.614778000	0.093892000
6	3.733662000	-0.348661000	0.026775000
6	3.239720000	0.981323000	-0.031566000
7	2.648453000	-1.216324000	-0.017307000
6	1.503998000	-0.452807000	-0.122735000
6	1.810737000	0.883556000	-0.113171000
6	0.742742000	1.872300000	-0.084182000
6	0.935565000	3.170196000	0.395788000
6	-0.113747000	4.077056000	0.476536000
6	-1.366132000	3.657867000	0.072105000
6	-1.599361000	2.377642000	-0.404951000
6	-0.550973000	1.464726000	-0.484708000
6	2.691965000	-2.675783000	0.062095000
6	3.350913000	-3.280879000	-1.169777000
6	3.313593000	-3.150463000	1.368264000
9	-2.399559000	4.513401000	0.141664000

6	0.103475000	-0.948320000	-0.193276000
6	-0.735920000	0.046310000	-1.009471000
6	-2.211483000	-0.338072000	-1.127722000
6	-2.540817000	-1.830582000	-1.246291000
6	-2.747219000	-2.624582000	0.042082000
6	-3.816281000	-2.013661000	0.947086000
6	-3.297425000	-0.876055000	1.774625000
8	-2.249633000	-0.850319000	2.369472000
8	-2.710221000	0.342916000	-2.257452000
8	-3.233023000	-3.919761000	-0.264047000
1	3.801823000	3.071737000	-0.127243000
1	6.220088000	2.601602000	0.021001000
1	7.049446000	0.272208000	0.154923000
1	5.488804000	-1.630918000	0.133032000
1	1.921197000	3.465656000	0.750219000
1	0.025683000	5.087333000	0.853498000
1	-2.597278000	2.129611000	-0.758242000
1	-3.711991000	0.864055000	2.346747000
1	1.640786000	-2.994867000	0.071443000
1	4.404551000	-2.987761000	-1.253065000
1	2.839638000	-2.951134000	-2.082505000
1	3.308692000	-4.376575000	-1.123835000
1	4.374852000	-2.885269000	1.438966000
1	3.234197000	-4.242178000	1.445400000
1	2.797968000	-2.704080000	2.226572000
1	0.053734000	-1.935823000	-0.672748000
1	-0.338458000	0.023012000	-2.042204000
1	-2.715119000	0.049332000	-0.226501000
1	-1.790097000	-2.333755000	-1.880616000

1	-3.492725000	-1.895049000	-1.795238000
1	-1.812455000	-2.699155000	0.624860000
1	-4.694727000	-1.709418000	0.362956000
1	-4.135641000	-2.802156000	1.643314000
1	-0.314571000	-1.059789000	0.823037000
1	-3.671024000	0.426808000	-2.108157000
1	-2.663133000	-4.295010000	-0.948849000
8	-4.154712000	0.181757000	1.807584000
8	-5.195832000	0.473696000	-0.920816000
1	-5.964284000	1.031408000	-1.091865000
1	-4.984960000	0.596923000	0.020387000

6. FLV (conformer B)

6	4.856593000	0.213681000	-0.910060000
6	5.847625000	-0.690128000	-1.243748000
6	5.632437000	-2.071188000	-1.109485000
6	4.424490000	-2.571702000	-0.653138000
6	3.419769000	-1.659375000	-0.314909000
6	3.633720000	-0.264870000	-0.421356000
7	2.125875000	-1.868808000	0.133752000
6	1.530465000	-0.623011000	0.322833000
6	2.424396000	0.379423000	-0.004225000
6	2.167168000	1.821056000	0.023082000
6	3.135196000	2.700702000	0.528412000
6	2.914900000	4.070302000	0.572191000
6	1.707829000	4.567098000	0.106459000
6	0.725984000	3.735003000	-0.405517000
6	0.965379000	2.367498000	-0.450209000
6	1.616936000	-3.136128000	0.671598000
6	1.392656000	-4.158339000	-0.432584000

6	2.490813000	-3.662535000	1.802498000
9	1.487278000	5.885073000	0.147264000
6	0.167300000	-0.408272000	0.774874000
6	-0.929115000	-1.103460000	0.446717000
6	-2.315591000	-0.728207000	0.880333000
6	-3.275692000	-0.721051000	-0.308982000
6	-4.719160000	-0.432337000	0.084855000
6	-5.663091000	-0.569953000	-1.093556000
6	-7.094653000	-0.466317000	-0.639560000
8	-7.839000000	0.276582000	-1.478046000
8	-7.551772000	-1.003088000	0.339606000
8	-2.343966000	0.510346000	1.579256000
8	-4.882217000	0.886320000	0.554368000
1	5.015678000	1.284917000	-1.030444000
1	6.803018000	-0.330589000	-1.621632000
1	6.425610000	-2.765944000	-1.380085000
1	4.272473000	-3.646125000	-0.580503000
1	4.068796000	2.293236000	0.914844000
1	3.657255000	4.758223000	0.970014000
1	-0.199269000	4.168222000	-0.778853000
1	0.217452000	1.704627000	-0.885926000
1	0.642710000	-2.887250000	1.108942000
1	2.331361000	-4.443089000	-0.923523000
1	0.722793000	-3.760999000	-1.205452000
1	0.942629000	-5.069629000	-0.018529000
1	3.482429000	-3.975957000	1.456228000
1	2.008817000	-4.531474000	2.268340000
1	2.629046000	-2.893385000	2.571950000
1	0.041109000	0.470424000	1.411383000

1	-0.864544000	-1.963531000	-0.225389000
1	-2.689582000	-1.459831000	1.617724000
1	-3.214718000	-1.698798000	-0.812824000
1	-2.941249000	0.036421000	-1.040133000
1	-5.032671000	-1.162748000	0.856769000
1	-5.444625000	0.201941000	-1.842020000
1	-5.536879000	-1.552989000	-1.570196000
1	-8.740192000	0.271403000	-1.108664000
1	-2.004054000	1.186720000	0.970105000
1	-4.262495000	0.993577000	1.295614000

7. TS₁ (pathway B)

6	-5.000849000	0.506590000	0.906940000
6	-6.133018000	-0.285981000	1.062960000
6	-6.084708000	-1.643918000	0.753063000
6	-4.906976000	-2.245870000	0.316531000
6	-3.769060000	-1.454001000	0.182290000
6	-3.820503000	-0.061334000	0.431620000
7	-2.478403000	-1.807274000	-0.187456000
6	-1.679135000	-0.659041000	-0.245366000
6	-2.499828000	0.474669000	0.168884000
6	-2.039193000	1.766506000	0.055056000
6	-2.894277000	2.895496000	-0.137679000
6	-2.394763000	4.111887000	-0.483812000
6	-0.980546000	4.283593000	-0.633950000
6	-0.096192000	3.302718000	-0.396415000
6	-0.565683000	1.984361000	0.066273000
6	-1.983899000	-3.142692000	-0.498142000
6	-2.229862000	-4.139815000	0.627355000
6	-2.500230000	-3.630063000	-1.844964000

9	-0.573058000	5.497903000	-1.033962000
6	-0.468084000	-0.560928000	-0.850014000
6	0.353509000	0.659285000	-0.798678000
6	1.647114000	0.551619000	0.001491000
6	2.600280000	-0.471848000	-0.615249000
6	4.026078000	-0.333785000	-0.100127000
6	4.893483000	-1.465316000	-0.628191000
6	6.348557000	-1.340198000	-0.292788000
8	7.008975000	-2.476187000	-0.551660000
8	1.344190000	0.208959000	1.327987000
8	4.028930000	-0.360457000	1.317542000
1	-5.037461000	1.560511000	1.176532000
1	-7.058099000	0.155834000	1.427890000
1	-6.979805000	-2.254421000	0.861347000
1	-4.894078000	-3.307304000	0.083531000
1	-3.971918000	2.749802000	-0.116534000
1	-3.041746000	4.956809000	-0.708114000
1	0.971338000	3.495396000	-0.492776000
1	-0.181292000	1.752346000	1.072165000
1	-0.894086000	-3.020712000	-0.568736000
1	-3.284230000	-4.420322000	0.726580000
1	-1.894379000	-3.729591000	1.586914000
1	-1.665275000	-5.059708000	0.428415000
1	-3.592924000	-3.737756000	-1.835604000
1	-2.067074000	-4.606977000	-2.096500000
1	-2.241065000	-2.919049000	-2.639699000
1	-0.136906000	-1.360966000	-1.517072000
1	0.620806000	1.019767000	-1.809959000
1	2.150644000	1.544372000	-0.040912000

1	2.609873000	-0.375685000	-1.713176000
1	2.215021000	-1.476429000	-0.375822000
1	4.435697000	0.631978000	-0.446936000
1	4.530739000	-2.422871000	-0.228223000
1	4.818629000	-1.546825000	-1.724028000
1	7.943956000	-2.310513000	-0.334590000
1	2.204534000	0.011996000	1.744053000
1	4.611943000	0.372417000	1.618973000
8	6.921691000	-0.357156000	0.130443000
8	5.789404000	1.712168000	1.618545000
1	6.401298000	1.196754000	1.059944000
1	6.253401000	1.840698000	2.454813000

8. B.II (pathway B)

6	-5.022721000	0.502378000	0.199082000
6	-6.121753000	-0.348530000	0.258538000
6	-5.949067000	-1.723500000	0.117199000
6	-4.687371000	-2.276608000	-0.079559000
6	-3.588727000	-1.422575000	-0.140666000
6	-3.747934000	-0.019542000	-0.009972000
7	-2.249425000	-1.736659000	-0.324390000
6	-1.503759000	-0.556268000	-0.310307000
6	-2.416868000	0.563371000	-0.084254000
6	-1.919414000	1.833350000	-0.000885000
6	-2.732908000	3.010435000	0.025153000
6	-2.198729000	4.255348000	-0.032670000
6	-0.775157000	4.407875000	-0.149636000
6	0.077403000	3.379736000	-0.099072000
6	-0.413674000	1.993153000	0.194190000
6	-1.651406000	-3.072641000	-0.317130000

6	-1.880097000	-3.782423000	1.009881000
6	-2.075604000	-3.889893000	-1.529200000
9	-0.336499000	5.658580000	-0.358712000
6	-0.196372000	-0.401231000	-0.589945000
6	0.458775000	0.941240000	-0.524174000
6	1.824491000	0.842081000	0.172887000
6	2.813494000	-0.048140000	-0.576208000
6	4.226651000	0.057981000	-0.036924000
6	5.197170000	-0.802745000	-0.834911000
6	6.596400000	-0.721328000	-0.300070000
8	7.500630000	-1.194731000	-1.163588000
8	1.606813000	0.369294000	1.492149000
8	4.209123000	-0.358965000	1.322789000
1	-5.176422000	1.571142000	0.329266000
1	-7.116080000	0.063990000	0.416521000
1	-6.813754000	-2.383763000	0.162712000
1	-4.575475000	-3.352630000	-0.182583000
1	-3.814004000	2.901343000	0.015755000
1	-2.817380000	5.149331000	-0.055549000
1	1.143333000	3.565671000	-0.216307000
1	-0.254753000	1.797313000	1.277148000
1	-0.568845000	-2.908027000	-0.383930000
1	-2.942498000	-3.967484000	1.212443000
1	-1.466005000	-3.183519000	1.829513000
1	-1.360066000	-4.748617000	1.007387000
1	-3.146942000	-4.126890000	-1.520859000
1	-1.526078000	-4.839634000	-1.551407000
1	-1.861143000	-3.345181000	-2.456823000
1	0.397885000	-1.244654000	-0.934722000

1	0.672565000	1.305520000	-1.553998000
1	2.265519000	1.858643000	0.222458000
1	2.819353000	0.226297000	-1.642729000
1	2.491496000	-1.097354000	-0.493712000
1	4.562214000	1.111963000	-0.091925000
1	4.877546000	-1.855698000	-0.785089000
1	5.202427000	-0.530170000	-1.898793000
1	8.368626000	-1.126755000	-0.725667000
1	2.493616000	0.248431000	1.880594000
1	5.119706000	-0.238567000	1.651057000
8	6.904038000	-0.289792000	0.792672000
8	1.350075000	-2.498933000	1.168741000
1	1.140781000	-1.559644000	1.336166000
1	2.216477000	-2.605779000	1.582017000

9. TS₂ (pathway B)

6	-4.855776000	0.566954000	-0.906653000
6	-6.026695000	-0.185658000	-0.959268000
6	-6.019156000	-1.537451000	-0.630548000
6	-4.833963000	-2.171001000	-0.254399000
6	-3.668935000	-1.417956000	-0.205845000
6	-3.659623000	-0.033692000	-0.513026000
7	-2.362495000	-1.815569000	0.109706000
6	-1.513792000	-0.730086000	0.003297000
6	-2.293807000	0.415919000	-0.360560000
6	-1.703222000	1.687237000	-0.305362000
6	-2.444271000	2.902326000	-0.399954000
6	-1.834123000	4.124579000	-0.333338000
6	-0.436920000	4.210412000	-0.163911000
6	0.328522000	3.094764000	-0.043287000

6	-0.282429000	1.793567000	0.000037000
6	-1.942538000	-3.143027000	0.541891000
6	-2.593262000	-3.529941000	1.863334000
6	-2.134068000	-4.186212000	-0.550707000
9	0.120701000	5.432115000	-0.123255000
6	-0.152359000	-0.674570000	0.278437000
6	0.546278000	0.539915000	-0.318542000
6	2.017908000	0.666705000	0.074228000
6	2.822451000	-0.583113000	-0.272681000
6	4.316061000	-0.324286000	-0.290358000
6	5.108297000	-1.573289000	-0.653263000
6	6.585676000	-1.311218000	-0.675860000
8	7.263570000	-2.265257000	-1.322318000
8	2.156766000	0.976954000	1.457004000
8	4.690242000	0.136650000	0.998199000
1	-4.887578000	1.614117000	-1.200876000
1	-6.955761000	0.291482000	-1.267113000
1	-6.941303000	-2.114497000	-0.671963000
1	-4.839409000	-3.231027000	-0.009889000
1	-3.521678000	2.855587000	-0.530081000
1	-2.408349000	5.046511000	-0.403142000
1	1.399917000	3.209396000	0.107797000
1	-0.393666000	1.606670000	1.399821000
1	-0.864004000	-3.055643000	0.726170000
1	-3.681704000	-3.624474000	1.771576000
1	-2.387551000	-2.770335000	2.627522000
1	-2.199125000	-4.491950000	2.215473000
1	-3.191691000	-4.332280000	-0.799920000
1	-1.729830000	-5.153379000	-0.224620000

1	-1.613075000	-3.883517000	-1.466981000
1	0.420342000	-1.601163000	0.325059000
1	0.582210000	0.452158000	-1.431541000
1	2.442933000	1.501363000	-0.519482000
1	2.512025000	-0.960052000	-1.259163000
1	2.606065000	-1.369209000	0.467786000
1	4.532984000	0.460387000	-1.041121000
1	4.917705000	-2.356698000	0.097126000
1	4.798843000	-1.985290000	-1.622947000
1	8.206546000	-2.026080000	-1.264837000
1	3.108541000	0.900703000	1.658733000
1	5.639799000	0.350122000	0.947346000
8	7.133724000	-0.355337000	-0.165591000
8	-0.294595000	0.976424000	2.486682000
1	0.689342000	1.042802000	2.548702000
1	-0.370555000	0.083500000	1.988138000

10. FP.1 (pathway B)

6	-5.015122000	0.219528000	-1.116498000
6	-6.069403000	-0.659581000	-1.294640000
6	-5.975904000	-1.989316000	-0.861975000
6	-4.824422000	-2.465692000	-0.254589000
6	-3.760125000	-1.580110000	-0.072514000
6	-3.844150000	-0.225698000	-0.490022000
7	-2.498832000	-1.786816000	0.473150000
6	-1.799548000	-0.600336000	0.382163000
6	-2.582194000	0.380810000	-0.173954000
6	-2.095950000	1.752767000	-0.240150000
6	-2.949593000	2.852327000	-0.354308000
6	-2.459482000	4.152591000	-0.336158000

6	-1.099317000	4.336336000	-0.178024000
6	-0.220767000	3.271079000	-0.053725000
6	-0.706130000	1.969964000	-0.093312000
6	-1.997888000	-3.018227000	1.080785000
6	-2.849805000	-3.448297000	2.266782000
6	-1.818235000	-4.117192000	0.042942000
9	-0.607149000	5.583018000	-0.134071000
6	-0.395074000	-0.363131000	0.811462000
6	0.200016000	0.752039000	-0.060845000
6	1.648574000	1.055932000	0.303272000
6	2.569212000	-0.152843000	0.129613000
6	4.034903000	0.233421000	0.097637000
6	4.933266000	-0.981227000	-0.088810000
6	6.381573000	-0.605875000	-0.117254000
8	7.168521000	-1.612884000	-0.555851000
8	1.679968000	1.539908000	1.623466000
8	4.334327000	0.891365000	1.317792000
1	-5.090483000	1.240939000	-1.485803000
1	-6.980216000	-0.316752000	-1.782590000
1	-6.815914000	-2.665368000	-1.011737000
1	-4.766152000	-3.505963000	0.058634000
1	-4.023821000	2.691287000	-0.420869000
1	-3.115313000	5.016042000	-0.417738000
1	0.832039000	3.485247000	0.108193000
1	-1.004709000	-2.761234000	1.473881000
1	-3.862161000	-3.738916000	1.963180000
1	-2.938959000	-2.634060000	2.995367000
1	-2.388421000	-4.310284000	2.765203000
1	-2.774019000	-4.410257000	-0.408439000

1	-1.375788000	-5.009240000	0.504594000
1	-1.157131000	-3.779534000	-0.764829000
1	-0.334200000	-0.072455000	1.873696000
1	0.216283000	0.356703000	-1.095519000
1	2.008408000	1.832434000	-0.406418000
1	2.327361000	-0.684752000	-0.804110000
1	2.410310000	-0.853238000	0.965442000
1	4.202447000	0.927745000	-0.748160000
1	4.787416000	-1.676025000	0.754136000
1	4.696377000	-1.544340000	-1.004773000
1	8.084091000	-1.279764000	-0.521020000
1	2.620159000	1.599003000	1.869444000
1	5.249790000	1.211012000	1.241150000
8	6.851430000	0.460285000	0.213201000
1	0.213330000	-1.271701000	0.694803000
8	5.526284000	-2.971673000	-2.600855000
1	6.307703000	-2.769398000	-2.065214000
1	5.316898000	-3.888203000	-2.385206000

11. FLV

6	4.801504000	0.658016000	0.725563000
6	5.944249000	-0.071779000	0.996743000
6	5.942812000	-1.471303000	0.887698000
6	4.806416000	-2.163946000	0.502311000
6	3.647668000	-1.428543000	0.231579000
6	3.633125000	-0.018154000	0.351232000
7	2.392046000	-1.830052000	-0.185633000
6	1.590566000	-0.700102000	-0.331488000
6	2.321782000	0.428776000	-0.014141000
6	1.899306000	1.833705000	-0.092355000

6	2.125998000	2.700418000	0.983558000
6	1.762177000	4.041459000	0.923038000
6	1.157738000	4.513523000	-0.229024000
6	0.913462000	3.688448000	-1.316102000
6	1.293536000	2.355963000	-1.243474000
6	1.923378000	-3.210766000	-0.318656000
6	2.591714000	-3.910047000	-1.493512000
6	2.051122000	-3.982058000	0.987806000
9	0.798327000	5.802167000	-0.296663000
6	0.206314000	-0.807151000	-0.770104000
6	-0.786196000	-0.047883000	-0.297833000
6	-2.193435000	-0.105123000	-0.794740000
6	-3.148753000	-0.457440000	0.351385000
6	-4.607322000	-0.229598000	0.007504000
6	-5.522251000	-0.591587000	1.170706000
6	-6.967932000	-0.361275000	0.842554000
8	-7.743432000	-0.356269000	1.932854000
8	-2.281933000	-1.026628000	-1.847530000
8	-4.921878000	-1.017016000	-1.127314000
1	4.803836000	1.745641000	0.793150000
1	6.857894000	0.442045000	1.290839000
1	6.854064000	-2.026895000	1.103245000
1	4.836671000	-3.246929000	0.406758000
1	2.582814000	2.308482000	1.891921000
1	1.933751000	4.720881000	1.754681000
1	0.446228000	4.102562000	-2.206619000
1	1.120291000	1.699063000	-2.094295000
1	0.851231000	-3.131210000	-0.538173000
1	3.675578000	-4.002363000	-1.350566000

1	2.422272000	-3.351760000	-2.422359000
1	2.180636000	-4.920021000	-1.617932000
1	3.096392000	-4.133668000	1.280417000
1	1.586653000	-4.970726000	0.881803000
1	1.546837000	-3.448778000	1.802377000
1	-0.037872000	-1.521956000	-1.558370000
1	-0.591943000	0.679787000	0.493938000
1	-2.464635000	0.917136000	-1.144869000
1	-2.900981000	0.144161000	1.239325000
1	-2.988473000	-1.515520000	0.613722000
1	-4.752230000	0.842210000	-0.232551000
1	-5.398406000	-1.659003000	1.412369000
1	-5.266974000	-0.032899000	2.081259000
1	-8.658099000	-0.226549000	1.622804000
1	-3.231502000	-1.170675000	-2.005013000
1	-5.843845000	-0.803930000	-1.359221000
8	-7.416673000	-0.203780000	-0.274351000

12. FLV

6	-4.602950000	0.352811000	-0.858911000
6	-5.773064000	-0.326941000	-1.144403000
6	-5.843003000	-1.722716000	-1.017590000
6	-4.751630000	-2.463804000	-0.593958000
6	-3.565771000	-1.780137000	-0.310929000
6	-3.476856000	-0.375849000	-0.455260000
7	-2.341140000	-2.239775000	0.147063000
6	-1.488430000	-1.159405000	0.298657000
6	-2.151272000	0.005543000	-0.059231000
6	-1.639635000	1.371989000	-0.010900000
6	-1.828132000	2.239905000	-1.101195000

6	-1.411564000	3.558508000	-1.046114000
6	-0.764706000	4.008594000	0.106475000
6	-0.462184000	3.156393000	1.165156000
6	-0.934693000	1.858155000	1.117205000
6	-1.942658000	-3.641267000	0.305843000
6	-2.675443000	-4.294578000	1.468079000
6	-2.073808000	-4.415586000	-0.998008000
9	-0.366798000	5.275063000	0.162379000
6	-0.115672000	-1.317627000	0.754744000
6	0.897136000	-0.611107000	0.244269000
6	2.289969000	-0.616195000	0.772658000
6	3.305160000	-0.868241000	-0.344656000
6	4.710948000	-0.478319000	0.058580000
6	5.711785000	-0.734097000	-1.059691000
6	7.107431000	-0.346756000	-0.670195000
8	7.926350000	-0.265242000	-1.726006000
8	2.399694000	-1.546996000	1.815040000
8	5.060257000	-1.222095000	1.214823000
1	-4.556838000	1.439349000	-0.915623000
1	-6.655704000	0.227099000	-1.458890000
1	-6.776354000	-2.235886000	-1.242981000
1	-4.837644000	-3.541738000	-0.477771000
1	-2.337725000	1.867767000	-1.988465000
1	-1.591174000	4.258506000	-1.858246000
1	0.043884000	3.554505000	2.041114000
1	-0.779568000	1.192243000	1.962903000
1	-0.874135000	-3.608031000	0.553842000
1	-3.757691000	-4.340139000	1.295142000
1	-2.507092000	-3.734831000	2.396084000

1	-2.313782000	-5.320332000	1.613398000
1	-3.117730000	-4.522492000	-1.314474000
1	-1.655789000	-5.422499000	-0.874522000
1	-1.526822000	-3.911538000	-1.803580000
1	0.092919000	-2.000604000	1.580498000
1	0.731517000	0.075832000	-0.588231000
1	2.483572000	0.416834000	1.149568000
1	3.023605000	-0.282572000	-1.230471000
1	3.271632000	-1.937099000	-0.609913000
1	4.714922000	0.604279000	0.293448000
1	5.718932000	-1.807302000	-1.307552000
1	5.435131000	-0.201457000	-1.979398000
1	8.806133000	-0.033212000	-1.377290000
1	3.350051000	-1.608643000	2.016635000
1	5.940242000	-0.905291000	1.486175000
8	7.488432000	-0.135525000	0.463051000
8	1.901311000	2.179887000	-1.078334000
1	1.442631000	2.354299000	-0.242632000
1	1.233980000	2.402351000	-1.740844000
8	-3.139020000	4.010984000	0.969539000
8	-3.441733000	2.832465000	1.142822000

13. TS₁

6	4.143047000	-1.806116000	-1.006621000
6	4.405674000	-3.171992000	-1.123522000
6	3.457266000	-4.100971000	-0.704726000
6	2.241967000	-3.704144000	-0.147630000
6	1.995512000	-2.340080000	-0.016097000
6	2.938420000	-1.401194000	-0.464814000
7	0.915048000	-1.657395000	0.567583000

6	1.089181000	-0.286770000	0.565735000
6	2.345906000	-0.037503000	-0.271679000
6	3.260395000	1.090377000	0.098447000
6	3.518702000	1.386905000	1.435944000
6	4.409253000	2.395344000	1.783310000
6	5.037826000	3.103747000	0.771483000
6	4.798358000	2.841432000	-0.567744000
6	3.902248000	1.830523000	-0.894805000
6	-0.323352000	-2.259897000	1.063639000
6	-1.119371000	-2.875392000	-0.078269000
6	-0.101764000	-3.216297000	2.225462000
9	5.894631000	4.079536000	1.098169000
6	1.276817000	0.211231000	-1.302028000
6	0.251734000	0.997997000	-0.837490000
6	-1.145684000	0.961713000	-1.366944000
6	-2.133698000	0.973601000	-0.201535000
6	-3.582321000	0.969003000	-0.646186000
6	-4.517272000	1.280422000	0.514910000
6	-5.959780000	1.060609000	0.181730000
8	-6.773251000	1.483553000	1.157422000
8	-1.305299000	-0.137278000	-2.225244000
8	-3.836269000	-0.316781000	-1.206650000
1	4.872715000	-1.066114000	-1.336017000
1	5.350068000	-3.512097000	-1.543946000
1	3.665898000	-5.164963000	-0.806813000
1	1.521351000	-4.450876000	0.175791000
1	2.998061000	0.821969000	2.208600000
1	4.622582000	2.643947000	2.820419000
1	5.307452000	3.429598000	-1.327857000

1	3.680351000	1.611183000	-1.940154000
1	-0.881271000	-1.397431000	1.456726000
1	-0.572924000	-3.705424000	-0.545868000
1	-1.313440000	-2.120532000	-0.852733000
1	-2.078424000	-3.265989000	0.283679000
1	0.383973000	-4.150578000	1.918458000
1	-1.073411000	-3.478670000	2.664042000
1	0.514972000	-2.750530000	3.003458000
1	1.035197000	-0.592802000	-1.995715000
1	0.468963000	1.853688000	-0.195857000
1	-1.309678000	1.910990000	-1.924545000
1	-1.945820000	1.870624000	0.402825000
1	-1.957917000	0.093711000	0.438233000
1	-3.728650000	1.742137000	-1.424371000
1	-4.272768000	0.663862000	1.392979000
1	-4.383464000	2.326872000	0.822139000
1	-7.680275000	1.281282000	0.865389000
1	-2.243229000	-0.403153000	-2.192164000
1	-4.777097000	-0.318870000	-1.467734000
8	-6.388197000	0.561183000	-0.840338000
8	-2.797060000	4.101922000	-0.467445000
1	-2.206961000	4.682614000	0.028256000
1	-2.922349000	4.551449000	-1.311964000
8	-4.334758000	-1.857883000	0.898649000
8	-3.523330000	-1.539121000	1.741697000

14. II

6	3.472894000	-1.201048000	1.633851000
6	4.859228000	-1.032800000	1.728991000
6	5.457243000	0.177074000	1.348980000

6	4.714253000	1.189745000	0.777127000
6	3.329182000	0.998957000	0.612967000
6	2.712783000	-0.196540000	1.079045000
7	2.394437000	1.860700000	0.072303000
6	1.147023000	1.183642000	0.152085000
6	1.253950000	-0.187737000	0.757775000
6	0.641242000	-1.473372000	0.313179000
6	1.174645000	-2.144164000	-0.789879000
6	0.617285000	-3.338382000	-1.224340000
6	-0.467307000	-3.858658000	-0.533523000
6	-1.002008000	-3.230072000	0.577759000
6	-0.432088000	-2.033160000	0.998425000
6	2.602415000	2.761312000	-1.077543000
6	3.577265000	3.888338000	-0.777066000
6	2.973309000	1.990691000	-2.335499000
9	-1.009835000	-5.010814000	-0.952214000
6	0.492731000	0.888688000	1.497160000
6	-0.203724000	1.684221000	0.419857000
6	-1.449094000	1.268500000	-0.353255000
6	-2.593156000	0.998887000	0.614837000
6	-3.873057000	0.566182000	-0.071729000
6	-5.067323000	0.633397000	0.866682000
6	-6.326803000	0.149969000	0.214883000
8	-7.413371000	0.406489000	0.956653000
8	-1.165219000	0.199865000	-1.209607000
8	-3.669005000	-0.760636000	-0.535209000
1	3.005289000	-2.137847000	1.932591000
1	5.472857000	-1.829889000	2.142458000
1	6.532316000	0.300599000	1.461030000

1	5.194322000	2.111567000	0.463411000
1	2.028854000	-1.707246000	-1.310162000
1	1.005361000	-3.872825000	-2.088306000
1	-1.847950000	-3.679586000	1.092394000
1	-0.831340000	-1.511409000	1.868786000
1	1.610576000	3.215409000	-1.223965000
1	4.621290000	3.556623000	-0.833812000
1	3.398205000	4.318602000	0.215802000
1	3.457515000	4.682036000	-1.525183000
1	3.950115000	1.503416000	-2.221301000
1	3.020422000	2.668479000	-3.198123000
1	2.226605000	1.213094000	-2.544924000
1	0.888943000	1.371151000	2.388221000
1	-0.225118000	2.754076000	0.673072000
1	-1.738952000	2.153874000	-0.963940000
1	-2.781852000	1.912452000	1.196991000
1	-2.292115000	0.207359000	1.320567000
1	-4.076152000	1.236747000	-0.929124000
1	-4.883513000	0.011425000	1.756784000
1	-5.221759000	1.663580000	1.213963000
1	-8.171979000	0.041510000	0.466515000
1	-1.907535000	-0.431293000	-1.172210000
1	-4.466462000	-0.994930000	-1.042173000
8	-6.398386000	-0.415981000	-0.857066000
8	-4.399879000	3.701172000	-0.047397000
1	-4.049075000	3.791043000	-0.941796000
1	-4.676526000	4.593324000	0.194628000
8	4.178862000	-0.683213000	-1.240288000
8	4.794468000	-1.594066000	-0.681213000

15. TS₂

6	-3.509997000	2.101358000	-1.387063000
6	-3.611597000	3.484899000	-1.279913000
6	-2.714255000	4.195923000	-0.483801000
6	-1.699199000	3.552797000	0.217338000
6	-1.600577000	2.174249000	0.091075000
6	-2.489885000	1.446151000	-0.716586000
7	-0.676614000	1.281913000	0.705741000
6	-1.029459000	0.043068000	0.356466000
6	-2.219188000	-0.015966000	-0.541316000
6	-3.394726000	-0.899486000	-0.212535000
6	-4.339757000	-0.484222000	0.730753000
6	-5.428995000	-1.282327000	1.049443000
6	-5.564295000	-2.507109000	0.412013000
6	-4.648036000	-2.950131000	-0.525992000
6	-3.563329000	-2.135846000	-0.833034000
6	0.322430000	1.581530000	1.754351000
6	1.385428000	2.586669000	1.348151000
6	-0.403431000	1.977763000	3.032877000
9	-6.611586000	-3.280060000	0.714078000
6	-0.982209000	-0.632320000	-1.195433000
6	-0.422442000	-1.276448000	0.078925000
6	1.035265000	-1.642622000	0.293355000
6	2.049644000	-0.878975000	-0.547739000
6	3.451519000	-1.015478000	0.001073000
6	4.458324000	-0.282946000	-0.874070000
6	5.859886000	-0.362743000	-0.345791000
8	6.674569000	0.519800000	-0.891354000
8	1.094256000	-3.029695000	0.052566000

8	3.772795000	-2.393987000	0.090808000
1	-4.220816000	1.531063000	-1.983991000
1	-4.398261000	4.014420000	-1.813460000
1	-2.807632000	5.277296000	-0.402367000
1	-1.010444000	4.124821000	0.832996000
1	-4.219072000	0.485103000	1.215765000
1	-6.173366000	-0.974770000	1.780044000
1	-4.791865000	-3.917818000	-1.000477000
1	-2.831766000	-2.470950000	-1.567883000
1	0.819712000	0.613699000	1.922189000
1	0.972355000	3.588508000	1.183489000
1	1.885111000	2.273245000	0.426665000
1	2.118751000	2.662025000	2.161528000
1	-0.945099000	2.923489000	2.905264000
1	0.318835000	2.111699000	3.847317000
1	-1.125865000	1.209087000	3.333581000
1	-0.889224000	-1.010597000	-2.209176000
1	-1.041841000	-2.102222000	0.467186000
1	1.261471000	-1.443437000	1.366314000
1	1.798157000	0.189763000	-0.615404000
1	2.009496000	-1.273835000	-1.574727000
1	3.479335000	-0.563574000	1.015823000
1	4.456355000	-0.730132000	-1.880713000
1	4.180902000	0.771830000	-1.008354000
1	7.588252000	0.376853000	-0.515463000
1	2.039717000	-3.260192000	0.090960000
1	4.667352000	-2.439669000	0.471907000
8	6.216897000	-1.176694000	0.502164000
8	0.595393000	1.717815000	-1.279715000

8	0.073871000	0.772172000	-1.986983000
8	8.848295000	-0.327176000	0.466115000
1	9.087610000	0.199502000	1.239376000
1	8.157076000	-0.942678000	0.780631000

16. 12

6	4.036887000	-0.154057000	-1.978701000
6	5.243387000	-0.838125000	-1.806795000
6	5.373496000	-1.761103000	-0.777500000
6	4.317465000	-2.035999000	0.095178000
6	3.111637000	-1.375146000	-0.089423000
6	2.973945000	-0.433962000	-1.145589000
7	1.920263000	-1.482280000	0.688265000
6	0.964409000	-0.868096000	-0.143187000
6	1.649228000	0.250494000	-0.909050000
6	1.896490000	1.575983000	-0.220586000
6	2.216300000	1.683980000	1.137078000
6	2.499307000	2.917948000	1.707174000
6	2.474490000	4.048721000	0.905851000
6	2.178001000	3.979534000	-0.444323000
6	1.889091000	2.736234000	-0.997128000
6	1.549505000	-2.635324000	1.528231000
6	1.694247000	-3.978237000	0.824157000
6	2.295425000	-2.585083000	2.853384000
9	2.742624000	5.240035000	1.452763000
6	0.218529000	0.240772000	-1.579958000
6	-0.347383000	-0.077393000	-0.140250000
6	-1.658060000	-0.801607000	0.032125000
6	-2.834052000	0.157939000	-0.110658000
6	-4.172238000	-0.550598000	-0.178652000

6	-5.325637000	0.434405000	-0.311357000
6	-6.655332000	-0.252898000	-0.339445000
8	-7.639807000	0.553255000	-0.758958000
8	-1.602976000	-1.371046000	1.325382000
8	-4.312044000	-1.325064000	1.002057000
1	3.929546000	0.595139000	-2.763152000
1	6.081180000	-0.640192000	-2.472325000
1	6.318288000	-2.284830000	-0.639791000
1	4.448150000	-2.760822000	0.895377000
1	2.238609000	0.784752000	1.752160000
1	2.743129000	3.017006000	2.762362000
1	2.177987000	4.888300000	-1.041452000
1	1.663527000	2.665770000	-2.062026000
1	0.480815000	-2.467941000	1.731011000
1	2.740199000	-4.212135000	0.588330000
1	1.125272000	-3.988414000	-0.112143000
1	1.312783000	-4.777806000	1.472500000
1	3.377102000	-2.725110000	2.725731000
1	1.936614000	-3.379378000	3.520357000
1	2.137559000	-1.620469000	3.351522000
1	-0.154938000	1.048439000	-2.216957000
1	-0.297816000	0.793876000	0.520683000
1	-1.745147000	-1.589459000	-0.737507000
1	-2.715706000	0.767001000	-1.021405000
1	-2.838095000	0.846937000	0.749625000
1	-4.174072000	-1.221168000	-1.060452000
1	-5.307709000	1.138614000	0.534192000
1	-5.222010000	1.061890000	-1.206472000
1	-8.459263000	0.027807000	-0.719931000

1	-2.503454000	-1.690592000	1.517106000
1	-5.158780000	-1.798857000	0.914139000
8	-6.863508000	-1.406277000	-0.018048000
8	0.681216000	-1.839085000	-1.225234000
8	0.115504000	-0.982143000	-2.255822000
8	-3.931227000	3.267863000	0.260114000
1	-3.014746000	3.383209000	0.539273000
1	-4.356563000	4.103761000	0.487144000

17. TS₃

6	4.063149000	-0.637469000	-2.428718000
6	5.420206000	-0.853538000	-2.181747000
6	5.872237000	-0.994722000	-0.875251000
6	4.998535000	-0.935884000	0.212361000
6	3.644028000	-0.750106000	-0.036414000
6	3.177109000	-0.609882000	-1.369858000
7	2.578372000	-0.649410000	0.896784000
6	1.433132000	-0.791654000	0.124785000
6	1.738583000	-0.218903000	-1.244468000
6	1.440063000	1.272310000	-1.170379000
6	2.236536000	2.152374000	-0.464008000
6	1.714159000	3.305587000	0.131919000
6	0.350989000	3.549191000	-0.022829000
6	-0.488158000	2.739339000	-0.749767000
6	0.001659000	1.476767000	-1.210857000
6	2.608113000	-0.938900000	2.332388000
6	3.081820000	-2.352225000	2.641635000
6	3.391480000	0.136610000	3.069687000
9	-0.160156000	4.662648000	0.527820000
6	0.366852000	-0.813839000	-1.559475000

6	-0.252750000	-0.021666000	-0.255170000
6	-1.520732000	-0.667884000	0.281972000
6	-2.741123000	-0.233930000	-0.531022000
6	-4.018495000	-0.959583000	-0.140616000
6	-5.228823000	-0.281061000	-0.770184000
6	-6.509345000	-0.980545000	-0.427507000
8	-7.508140000	-0.660169000	-1.257460000
8	-1.616207000	-0.240242000	1.634740000
8	-4.140573000	-0.944400000	1.270872000
1	3.700387000	-0.496789000	-3.445685000
1	6.123873000	-0.901246000	-3.010037000
1	6.932766000	-1.154523000	-0.687004000
1	5.381352000	-1.045043000	1.224438000
1	3.294300000	1.920976000	-0.328747000
1	2.333099000	4.010692000	0.679400000
1	-1.531571000	3.015986000	-0.877916000
1	-0.558573000	1.148246000	-2.092970000
1	1.551178000	-0.856041000	2.632557000
1	4.127211000	-2.505371000	2.344732000
1	2.469307000	-3.089775000	2.109830000
1	3.007676000	-2.549178000	3.718665000
1	4.458613000	0.112797000	2.812466000
1	3.308109000	-0.003736000	4.154541000
1	3.004085000	1.130305000	2.811815000
1	-0.163168000	-0.683178000	-2.509530000
1	0.017608000	0.681919000	0.536441000
1	-1.434920000	-1.767869000	0.250434000
1	-2.563284000	-0.419693000	-1.602859000
1	-2.882254000	0.848613000	-0.392445000

1	-3.963521000	-2.008768000	-0.490360000
1	-5.288641000	0.746925000	-0.376509000
1	-5.136728000	-0.199311000	-1.861374000
1	-8.299095000	-1.130163000	-0.936049000
1	-2.466408000	-0.596353000	1.961062000
1	-4.970147000	-1.412204000	1.478645000
8	-6.659389000	-1.748510000	0.501637000
8	1.133467000	-2.174759000	-0.047293000
8	0.342135000	-2.158241000	-1.246620000
8	-2.930439000	2.370736000	1.360808000
1	-2.403192000	1.587565000	1.605584000
1	-2.297456000	3.099605000	1.390680000

18. I3

6	4.439981000	0.303044000	-1.358482000
6	5.434979000	-0.555961000	-1.818090000
6	5.465283000	-1.883137000	-1.406015000
6	4.494414000	-2.385021000	-0.541167000
6	3.511663000	-1.521219000	-0.082341000
6	3.477558000	-0.159451000	-0.462548000
7	2.419471000	-1.801694000	0.743429000
6	1.612465000	-0.688443000	0.859493000
6	2.286704000	0.427277000	0.145192000
6	1.815517000	1.719535000	0.148573000
6	0.393666000	2.037475000	0.584139000
6	0.132034000	3.473590000	0.897469000
6	0.993675000	4.419884000	0.516690000
6	2.243482000	4.106368000	-0.115672000
6	2.628953000	2.819836000	-0.295779000
6	2.046558000	-3.087693000	1.339431000

6	1.594220000	-4.078624000	0.277446000
6	3.135292000	-3.624371000	2.256781000
9	0.755591000	5.720216000	0.728463000
6	-0.041945000	0.673974000	-1.530673000
6	-0.675401000	1.578781000	-0.503417000
6	-1.916776000	0.994178000	0.162687000
6	-3.042429000	0.673071000	-0.819933000
6	-4.107950000	-0.191066000	-0.170773000
6	-5.226447000	-0.540594000	-1.142928000
6	-6.281073000	-1.398401000	-0.507727000
8	-7.063042000	-1.996284000	-1.416658000
8	-2.342544000	1.945278000	1.114887000
8	-4.634794000	0.527047000	0.937614000
1	4.416578000	1.319915000	-1.740757000
1	6.184127000	-0.183731000	-2.513766000
1	6.244485000	-2.548607000	-1.772841000
1	4.507105000	-3.432467000	-0.253399000
1	0.158406000	1.422949000	1.464096000
1	-0.818795000	3.713039000	1.365111000
1	2.892515000	4.933873000	-0.395987000
1	3.625208000	2.625624000	-0.676374000
1	1.177181000	-2.834681000	1.961219000
1	2.374206000	-4.262558000	-0.472927000
1	0.694059000	-3.704379000	-0.225412000
1	1.342703000	-5.038611000	0.745983000
1	4.019068000	-3.974318000	1.709381000
1	2.744121000	-4.478409000	2.823263000
1	3.459565000	-2.859012000	2.971934000
1	0.686530000	1.187940000	-2.200662000

1	-0.966900000	2.487411000	-1.063137000
1	-1.621247000	0.054510000	0.658006000
1	-2.655383000	0.131545000	-1.693586000
1	-3.489575000	1.618272000	-1.171236000
1	-3.626004000	-1.123306000	0.177583000
1	-5.714561000	0.384005000	-1.490496000
1	-4.843144000	-1.050429000	-2.036914000
1	-7.723768000	-2.508442000	-0.916427000
1	-3.193470000	1.611175000	1.456727000
1	-5.243052000	-0.084136000	1.388082000
8	-6.447313000	-1.546644000	0.685111000
8	0.551759000	-0.674433000	1.481799000
8	-0.273564000	-0.503770000	-1.689672000
8	-1.399229000	-2.388593000	0.270641000
1	-0.874864000	-1.980675000	0.980628000
1	-1.108446000	-1.875588000	-0.502168000

19. TS₄

6	-1.535992000	-0.152379000	2.651257000
6	-2.300823000	-0.922178000	3.530805000
6	-3.311064000	-1.741407000	3.042862000
6	-3.596769000	-1.806750000	1.677521000
6	-2.836327000	-1.034745000	0.811761000
6	-1.800809000	-0.213992000	1.295148000
7	-2.951178000	-0.872558000	-0.578368000
6	-2.111108000	0.136185000	-1.005809000
6	-1.138617000	0.414086000	0.113310000
6	-0.679653000	1.818660000	0.208257000
6	-1.410403000	2.985263000	0.064622000
6	-0.739751000	4.201486000	0.108263000

6	0.647375000	4.255100000	0.286907000
6	1.412718000	3.125572000	0.422053000
6	0.760319000	1.861790000	0.275544000
6	-3.949372000	-1.455842000	-1.476806000
6	-3.876627000	-2.974255000	-1.483774000
6	-5.340394000	-0.916237000	-1.181219000
9	1.217733000	5.455562000	0.353648000
6	0.302664000	-0.355566000	-0.235296000
6	1.245712000	0.469990000	0.696031000
6	2.719222000	0.167258000	0.493655000
6	3.053859000	-1.198589000	1.090909000
6	4.361838000	-1.850918000	0.641984000
6	4.439567000	-2.209486000	-0.858421000
6	3.060204000	-2.347758000	-1.455528000
8	2.250448000	-3.175331000	-1.100368000
8	3.464097000	1.193330000	1.155672000
8	4.554786000	-3.059080000	1.346642000
1	-0.757442000	0.506615000	3.035967000
1	-2.105028000	-0.876199000	4.599930000
1	-3.902337000	-2.340182000	3.733143000
1	-4.405018000	-2.438526000	1.317599000
1	-2.488793000	2.950905000	-0.075975000
1	-1.275497000	5.142919000	0.002957000
1	-3.641866000	-1.088829000	-2.465301000
1	-4.207171000	-3.415243000	-0.535175000
1	-2.853466000	-3.315193000	-1.678879000
1	-4.527229000	-3.369643000	-2.273552000
1	-5.351303000	0.178144000	-1.255821000
1	-5.683177000	-1.194460000	-0.176196000

1	-6.062757000	-1.315570000	-1.904093000
1	0.167919000	-1.405676000	0.098192000
1	1.008894000	0.321837000	1.763114000
1	2.928949000	0.192706000	-0.587344000
1	2.250208000	-1.920218000	0.892816000
1	3.094491000	-1.053161000	2.184369000
1	5.203050000	-1.158406000	0.856125000
1	5.000321000	-1.446718000	-1.409715000
1	4.981707000	-3.159557000	-0.922353000
1	1.819937000	-1.148461000	-2.242135000
1	4.396506000	1.063920000	0.936207000
1	4.333829000	-2.905959000	2.275426000
8	2.798289000	-1.364045000	-2.317615000
8	-2.156040000	0.676145000	-2.098332000
8	0.637340000	-0.189420000	-1.502079000
1	0.734379000	1.717876000	-0.945966000
1	2.486268000	3.170746000	0.581005000
8	0.241902000	2.228895000	-2.707212000
1	0.663470000	1.354376000	-2.786944000
1	-0.691386000	1.944135000	-2.649514000

20. FP2

6	-2.824019000	0.611374000	2.610556000
6	-3.958301000	0.217126000	3.323891000
6	-4.901847000	-0.608983000	2.724123000
6	-4.752886000	-1.054476000	1.408628000
6	-3.623849000	-0.651349000	0.708795000
6	-2.662412000	0.172587000	1.309855000
7	-3.239446000	-0.925416000	-0.616119000
6	-2.058440000	-0.283361000	-0.923371000

6	-1.532358000	0.386776000	0.353902000
6	-1.030210000	1.778037000	0.080987000
6	-1.755097000	2.959766000	-0.004882000
6	-1.088495000	4.134536000	-0.334727000
6	0.279186000	4.087964000	-0.578494000
6	1.020107000	2.919810000	-0.492934000
6	0.346651000	1.755834000	-0.150752000
6	-3.960913000	-1.709442000	-1.621074000
6	-4.065434000	-3.170978000	-1.213032000
6	-5.301491000	-1.080962000	-1.968771000
9	0.905124000	5.224791000	-0.899458000
6	-0.210734000	-0.294199000	0.833241000
6	0.925802000	0.383285000	0.048988000
6	1.336567000	-0.353538000	-1.269291000
6	2.769562000	-0.843219000	-1.191483000
6	3.006158000	-1.872403000	-0.091929000
6	4.452241000	-2.325877000	-0.054308000
6	5.402606000	-1.284619000	0.456982000
8	5.056900000	-0.227742000	0.965370000
8	1.226091000	0.467414000	-2.402886000
8	2.225785000	-3.033217000	-0.290878000
1	-2.077926000	1.267149000	3.061518000
1	-4.104431000	0.558320000	4.346409000
1	-5.783307000	-0.914414000	3.285104000
1	-5.511264000	-1.691078000	0.960469000
1	-2.827683000	2.968930000	0.188421000
1	-1.605002000	5.088237000	-0.410771000
1	-3.309520000	-1.642929000	-2.502926000
1	-4.712480000	-3.317268000	-0.338974000

1	-3.075098000	-3.579038000	-0.977654000
1	-4.489166000	-3.757401000	-2.037615000
1	-5.998348000	-1.088014000	-1.121295000
1	-5.772281000	-1.636746000	-2.789151000
1	-5.170563000	-0.041576000	-2.292077000
1	-0.108748000	-0.010187000	1.896316000
1	1.817715000	0.454660000	0.691759000
1	0.681708000	-1.228601000	-1.388769000
1	3.433621000	0.023888000	-1.046651000
1	3.022081000	-1.301653000	-2.159243000
1	2.773346000	-1.425753000	0.892539000
1	4.535975000	-3.206444000	0.599177000
1	4.786417000	-2.663380000	-1.046059000
1	-0.817658000	-2.060129000	1.368984000
1	0.272041000	0.521206000	-2.587889000
1	1.317492000	-2.802042000	-0.035182000
8	6.670098000	-1.650728000	0.316081000
8	-1.544361000	-0.267300000	-2.027016000
8	-0.203338000	-1.699466000	0.713340000
1	7.242628000	-0.929651000	0.695024000
1	2.088306000	2.929480000	-0.698944000
8	7.630982000	0.623749000	1.445956000
1	7.893108000	1.287519000	0.795333000
1	6.657437000	0.707907000	1.510968000

21. Model FLV

6	-4.248620000	-0.265549000	-0.107581000
6	-3.576284000	0.928231000	-0.066239000
7	-3.312159000	-1.259355000	-0.090292000
6	-2.037635000	-0.734271000	-0.018105000

6	-2.179846000	0.656101000	-0.025872000
6	-1.184380000	1.721905000	-0.055511000
6	0.047655000	1.684987000	-0.568941000
6	-0.936001000	-1.668037000	0.121224000
6	0.297954000	-1.433093000	0.577135000
1	0.456817000	0.786111000	-1.027535000
1	-1.192228000	-2.697768000	-0.150089000
1	0.619102000	-0.441647000	0.888260000
1	1.021718000	-2.239681000	0.661770000
1	-5.306476000	-0.488855000	-0.155575000
1	-4.021729000	1.916784000	-0.096242000
1	-3.512582000	-2.247834000	-0.032490000
1	-1.544407000	2.673186000	0.347488000
1	0.684700000	2.566575000	-0.562831000

22. CI/AC

6	-4.248620000	-0.265549000	-0.107581000
6	-3.576284000	0.928231000	-0.066239000
7	-3.312159000	-1.259355000	-0.090292000
6	-2.037635000	-0.734271000	-0.018105000
6	-2.179846000	0.656101000	-0.025872000
6	-1.184380000	1.721905000	-0.055511000
6	0.047655000	1.684987000	-0.568941000
6	-0.936001000	-1.668037000	0.121224000
6	0.297954000	-1.433093000	0.577135000
1	0.456817000	0.786111000	-1.027535000
1	-1.192228000	-2.697768000	-0.150089000
1	0.619102000	-0.441647000	0.888260000
1	1.021718000	-2.239681000	0.661770000
1	-5.306476000	-0.488855000	-0.155575000

1	-4.021729000	1.916784000	-0.096242000
1	-3.425687000	-2.325029000	0.310484000
1	-1.544407000	2.673186000	0.347488000
1	0.684700000	2.566575000	-0.562831000

23. Model TS

6	2.443601000	0.025290000	0.012824000
6	1.686272000	1.155401000	-0.011655000
7	1.615593000	-1.072132000	0.058590000
6	0.291405000	-0.671361000	0.112058000
6	0.304973000	0.767352000	0.072308000
6	-0.847690000	1.499449000	-0.232816000
6	-2.115639000	1.072429000	0.159384000
6	-0.801356000	-1.469099000	-0.232986000
6	-2.109728000	-1.096676000	0.084533000
1	-2.275268000	0.907632000	1.218652000
1	-0.623670000	-2.251005000	-0.976937000
1	-2.912982000	-1.548080000	-0.503830000
1	-2.379115000	-0.995519000	1.128565000
1	3.520279000	-0.096267000	0.021908000
1	2.057076000	2.172859000	-0.047352000
1	1.918632000	-2.031157000	0.128767000
1	-0.746276000	2.303555000	-0.966197000
1	-2.983033000	1.522752000	-0.329061000

24. Model A.II

6	-4.319396000	-0.239430000	-0.123997000
6	-3.685415000	0.948832000	-0.033711000
7	-3.420754000	-1.299304000	-0.239337000
6	-2.126262000	-0.788104000	-0.081727000
6	-2.258039000	0.679554000	-0.052581000

6	-1.160683000	1.456662000	-0.112126000
6	0.181091000	0.801453000	-0.287786000
6	-0.954086000	-1.419830000	0.080310000
6	0.256220000	-0.573994000	0.374841000
1	0.376097000	0.690032000	-1.372589000
1	-0.886691000	-2.506135000	0.127738000
1	0.347821000	-0.444224000	1.470928000
1	1.175535000	-1.082563000	0.055169000
1	-5.384773000	-0.441370000	-0.159939000
1	-4.154483000	1.925143000	-0.017694000
1	-3.657633000	-2.232866000	0.065489000
1	-1.239061000	2.542607000	-0.152027000
1	0.986112000	1.441328000	0.097613000